ABSTRACT:

Similarity based Virtual Screening (VS) deals with a large amount of data containing irrelevant and/or redundant fragments or features. Recent use of Bayesian network as an alternative for existing tools for similarity based VS has received noticeable attention of the researchers in the field of chemoinformatics. Approach: To this end, different models of Bayesian network have been developed. In this study, we enhance the Bayesian Inference Network (BIN) using a subset of selected molecule's features. Results: In this approach, a few features were filtered from the molecular fingerprint features based on a features selection approach. Conclusion: Simulated virtual screening experiments with MDL Drug Data Report (MDDR) data sets showed that the proposed method provides simple ways of enhancing the cost effectiveness of ligand-based virtual screening searches, especially for higher diversity data set.